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ACYCLIC ORIENTATIONS OF GRAPHS*

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Abstract. Let G be a finite graph with p vertices and χ its chromatic polynomial. A combinatorial interpretation is given to the positive integer $(-1)^p \chi(-\lambda)$, where λ is a positive integer, in terms of acyclic orientations of G. In particular, $(-1)^p \chi(-1)$ is the number of acyclic orientations of G. An application is given to the enumeration of labeled acyclic digraphs. An algebra of full binomial type, in the sense of Doubilet–Rota–Stanley, is constructed which yields the generating functions which occur in the above context.

1. The chromatic polynomial with negative arguments

Let G be a finite graph, which we assume to be without loops or multiple edges. Let $V = V(G)$ denote the set of vertices of G and $X = X(G)$ the set of edges. An edge $e \in X$ is thought of as an unordered pair $\{u, v\}$ of two distinct vertices. The integers p and q denote the cardinalities of V and X, respectively. An *orientation* of G is an assignment of a direction to each edge $\{u, v\}$, denoted by $u \to v$ or $v \to u$, as the case may be. An orientation of G is said to be *acyclic* if it has no directed cycles.

Let $\chi(\lambda) = \chi(G, \lambda)$ denote the chromatic polynomial of G evaluated at $\lambda \in \mathbf{C}$. If λ is a non-negative integer, then $\chi(\lambda)$ has the following rather unorthodox interpretation.

Proposition 1.1. $\chi(\lambda)$ *is equal to the number of pairs* $(\sigma, \mathcal{O})$, *where* σ *is any map* $\sigma : V \to \{1, 2, ..., \lambda\}$ *and* $\mathcal{O}$ *is an orientation of* G, *subject to the two conditions:*

(a) *The orientation* $\mathcal{O}$ *is acyclic.*

(b) *If* $u \to v$ *in the orientation* $\mathcal{O}$, *then* $\sigma(u) > \sigma(v)$.

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Proof. Condition (b) forces the map σ to be a proper coloring (i.e., if $\{u, v\} \in X$, then $\sigma(u) \neq \sigma(v)$). From (b), condition (a) follows automatically. Conversely, if σ is proper, then (b) defines a unique acyclic orientation of G. Hence, the number of allowed σ is just the number of proper colorings of G with the colors $1, 2, \ldots, \lambda$, which by definition is $\chi(\lambda)$.

Proposition 1.1 suggests the following modification of $\chi(\lambda)$. If λ is a non-negative integer, define $\bar{\chi}(\lambda)$ to be the number of pairs $(\sigma, \mathcal{O})$, where σ is any map $\sigma: V \to \{1, 2, \ldots, \lambda\}$ and $\mathcal{O}$ is an orientation of G, subject to the two conditions:

(a′) The orientation $\mathcal{O}$ is acyclic,

(b′) If $u \to v$ in the orientation $\mathcal{O}$, then $\sigma(u) \geq \sigma(v)$. We then say that σ is *compatible* with $\mathcal{O}$.

The relationship between χ and $\bar{\chi}$ is somewhat analogous to the relationship between combinations of n things taken k at a time without repetition, enumerated by $\binom{n}{k}$, and with repetition, enumerated by $\binom{n+k-1}{k} = (-1)^k \binom{-n}{k}$.

Theorem 1.2. *For all non-negative integers* λ,

$$\bar{\chi}(\lambda) = (-1)^p \chi(-\lambda).$$

Proof. Recall the well-known fact that the chromatic polynomial $\chi(G, \lambda)$ is uniquely determined by the three conditions:

(i) $\chi(G_0, \lambda) = \lambda$, where G_0 is the one-vertex graph.

(ii) $\chi(G + H, \lambda) = \chi(G, \lambda)\, \chi(H, \lambda)$, where $G + H$ is the disjoint union of G and H,

(iii) for all $e \in X$, $\chi(G, \lambda) = \chi(G \backslash e, \lambda) - \chi(G/e, \lambda)$, where $G \backslash e$ denotes G with the edge e deleted and G/e denotes G with the edge e contracted to a point.

Hence, it suffices to prove the following three properties of $\bar{\chi}$:

(i′) $\bar{\chi}(G_0, \lambda) = \lambda$, where G_0 is the one-vertex graph,

(ii′) $\bar{\chi}(G + H, \lambda) = \bar{\chi}(G, \lambda)\, \bar{\chi}(H, \lambda)$,

(iii′) $\bar{\chi}(G, \lambda) = \bar{\chi}(G \backslash e, \lambda) + \bar{\chi}(G/e, \lambda)$.

Properties (i′) and (ii′) are obvious, so we need only prove (iii′). Let $\sigma: V(G \backslash e) \to \{1, 2, \ldots, \lambda\}$ and let $\mathcal{O}$ be an acyclic orientation of $G \backslash e$ compatible with σ, where $e = \{u, v\} \in X$. Let $\mathcal{O}_1$ be the orientation of G obtained by adjoining $u \to v$ to $\mathcal{O}$, and $\mathcal{O}_2$ that obtained by adjoining $v \to u$. Observe that σ is defined on $V(G)$ since $V(G) = V(G \backslash e)$. We will show that for each pair (σ, O), exactly one of O_1 and O_2 is an acyclic orientation compatible with σ, except for $\bar{\chi}(G/e, \lambda)$ of these pairs, in which case both O_1 and O_2 are acyclic orientations compatible with σ. It then follows that $\bar{\chi}(G, \lambda) = \bar{\chi}(G\backslash e, \lambda) + \bar{\chi}(G/e, \lambda)$, so proving the theorem.

For each pair (σ, O), where $\sigma : G\backslash e \to \{1, 2, \ldots, \lambda\}$ and O is an acyclic orientation of $G\backslash e$ compatible with σ, one of the following three possibilities must hold.

Case 1: $\sigma(u) > \sigma(v)$. Clearly O_2 is not compatible with σ while O_1 is compatible. Moreover, O_1 is acyclic, since if $u \to v \to w_1 \to w_2 \to \ldots \to u$ were a directed cycle in O_1, we would have $\sigma(u) > \sigma(v) \geqslant \sigma(w_1) \geqslant \sigma(w_2) \geqslant \ldots \geqslant \sigma(u)$, which is impossible.

Case 2: $\sigma(u) < \sigma(v)$. Then symmetrically to Case 1, O_2 is acyclic and compatible with σ, while O_1 is not compatible.

Case 3: $\sigma(u) = \sigma(v)$. Both O_1 and O_2 are compatible with σ. We claim that at least one of them is acyclic. Suppose not. Then O_1 contains a directed cycle $u \to v \to w_1 \to w_2 \to \ldots \to u$ while O_2 contains a directed cycle $v \to u \to w_1' \to w_2' \to \ldots \to v$. Hence, O contains the directed cycle

$$u \to w_1' \to w_2' \to \ldots \to v \to w_1 \to w_2 \to \ldots \to u,$$

contradicting the assumption that O is acyclic.

It remains to prove that both O_1 and O_2 are acyclic for exactly $\bar{\chi}(G/e, \lambda)$ pairs (σ, O), with $\sigma(u) = \sigma(v)$. To do this we define a bijection $\Phi(\sigma, O) = (\sigma', O')$ between those pairs (σ, O) such that both O_1 and O_2 are acyclic (with $\sigma(u) = \sigma(v)$) and those pairs (σ', O') such that $\sigma' : G/e \to \{1, 2, \ldots, \lambda\}$ and O' is an acyclic orientation of G/e compatible with σ'. Let z be the vertex of G/e obtained by identifying u and v, so

$$V(G/e) = V(G\backslash e) - \{u, v\} \cup \{z\}$$

and $X(G/e) = X(G\backslash e)$. Given (σ, O), define σ' by $\sigma'(w) = \sigma(w)$ for all $w \in V(G\backslash e) - \{z\}$ and $\sigma'(z) = \sigma(u) = \sigma(v)$. Define O' by $w_1 \to w_2$ in O' if and only if $w_1 \to w_2$ in O. It is easily seen that the map $\Phi(\sigma, O) = (\sigma', O')$ establishes the desired bijection, and we are through.

Theorem 1.2 provides a combinatorial interpretation of the positive integer $(-1)^p \chi(G, -\lambda)$, where λ is a positive integer. In particular, when $\lambda = 1$ every orientation of G is automatically compatible with every map $\sigma : G \to \{1\}$. We thus obtain the following corollary.

Corollary 1.3. *If G is a graph with p vertices, then $(-1)^p \chi(G, -1)$ is equal to the number of acyclic orientations of G.*

In [5], the following question was raised (for a special class of graphs). Let G be a p-vertex graph and let ω be a *labeling* of G, i.e., a bijection $\omega : V(G) \to \{1, 2, ..., p\}$. Define an equivalence relation $\sim$ on the set of all $p!$ labelings ω of G by the condition that $\omega \sim \omega'$ if whenever $\{u, v\} \in X(G)$, then $\omega(u) < \omega(v) \Leftrightarrow \omega'(u) < \omega'(v)$. How many equivalence classes of labelings of G are there? Clearly two labelings ω and ω' are equivalent if and only if the unique orientations $\mathcal{O}$ and $\mathcal{O}'$ compatible with ω and ω', respectively, are equal. Moreover, the orientations $\mathcal{O}$ which arise in this way are precisely the acyclic ones. Hence, by Corollary 1.3, the number of equivalence classes is $(-1)^p \chi(G, -1)$.

We conclude this section by discussing the relationship between the chromatic polynomial of a graph and the order polynomial [4;5;6] of a partially ordered set. If P is a p-element partially ordered set, define the *order polynomial* $\Omega(P, \lambda)$ (evaluated at the non-negative integer λ) to be the number of order-preserving maps $\sigma : P \to \{1, 2, ..., \lambda\}$. Define the *strict order polynomial* $\bar{\Omega}(P, \lambda)$ to be the number of *strict* order-preserving maps $\sigma : P \to \{1, 2, ..., \lambda\}$, i.e., if $x < y$ in P, then $\sigma(x) < \sigma(y)$. In [5], it was shown that Ω and $\bar{\Omega}$ are polynomials in λ related by $\bar{\Omega}(P, \lambda) = (-1)^p \Omega(P, -\lambda)$. This is the precise analogue of Theorem 1.2. We shall now clarify this analogy.

If $\mathcal{O}$ is an orientation of a graph G, regard $\mathcal{O}$ as a binary relation $\geqslant$ on $V(G)$ defined by $u \geqslant v$ if $u \to v$. If $\mathcal{O}$ is acyclic, then the transitive and reflexive closure $\bar{\mathcal{O}}$ of $\mathcal{O}$ is a partial ordering of $V(G)$. Moreover, a map $\sigma : V(G) \to \{1, 2, ..., \lambda\}$ is compatible with $\mathcal{O}$ if and only if σ is order-preserving when considered as a map from $\bar{\mathcal{O}}$. Hence the number of σ compatible with $\mathcal{O}$ is just $\Omega(\bar{\mathcal{O}}, \lambda)$ and we conclude that

$$\bar{\chi}(G, \lambda) = \sum_{\mathcal{O}} \Omega(\bar{\mathcal{O}}, \lambda),$$

where the sum is over all acyclic orientations $\mathcal{O}$ of G. In the same way, using Proposition 1.1, we deduce

$$(1) \qquad \chi(G, \lambda) = \sum_{\mathcal{O}} \bar{\Omega}(\bar{\mathcal{O}}, \lambda).$$

Hence, Theorem 1.2 follows from the known result $\bar{\Omega}(P, \lambda) = (-1)^p \Omega(P, -\lambda)$, but we thought a direct proof to be more illuminating. Equation (1) strengthens the claim made in [4] that the strict order polynomial $\bar{\Omega}$ is a partially-ordered set analogue of the chromatic polynomial χ.

2. Enumeration of labeled acyclic digraphs

Corollary 1.3, when combined with a result of Read (also obtained by Bender and Goldman), yields an immediate solution to the problem of enumerating labeled acyclic digraphs with n vertices. The same result was obtained by R.W. Robinson (to be published), who applies it to the unlabeled case.

Proposition 2.1. *Let $f(n)$ be the number of labeled acyclic digraphs with n vertices. Then*

$$\sum_{n=0}^{\infty} f(n)\, x^n/n!\; 2^{\binom{n}{2}} = \left(\sum_{n=0}^{\infty} (-1)^n x^n/n!\, 2^{\binom{n}{2}} \right)^{-1}.$$

Proof. By Corollary 1.3,

$$f(n) = (-1)^n \sum_G \chi(G, -1), \tag{2}$$

where the sum is over all labeled graphs G with n vertices. Now, Read [3] (see also [1]) has shown that if

$$M_n(k) = \sum_G \chi(G, k)$$

(where the sum has the same range as in (2)), then

$$\sum_{n=0}^{\infty} M_n(k)\, x^n/n!\; 2^{\binom{n}{2}} = \left(\sum_{n=0}^{\infty} x^n/n!\; 2^{\binom{n}{2}} \right)^k. \tag{3}$$

Actually, the above papers have $2^{n^2/2}$ where we have $2^{\binom{n}{2}}$ – this amounts to the transformation $x' = 2^{1/2}x$. One advantage of our 'normalization' is that the numbers $n!\,2^{\binom{n}{2}}$ are integers; a second is that the function

$$F(x) = \sum_{n=0}^{\infty} x^n/n!\,2^{\binom{n}{2}}$$

satisfies the functional relation $F'(x) = F(\frac{1}{2}x)$. A third advantage is mentioned in the next section. Thus setting $k = -1$ and changing x to $-x$ in (3) yields the desired result.

By analyzing the behavior of the function $F(x) = \Sigma_{n=0}^{\infty} x^n/n!\,2^{\binom{n}{2}}$, we obtain estimates for $f(n)$. For instance, Rouché's theorem can be used to show that $F(x)$ has a unique zero $\alpha \approx -1.488$ satisfying $|\alpha| \leqslant 2$. Standard techniques yield the asymptotic formula

$$f(n) \sim C 2^{\binom{n}{2}} n!(-\alpha)^{-n},$$

where α is as above and $1.741 \approx C = 1/\alpha F(\frac{1}{2}\alpha)$. A more careful analysis of $F(x)$ will yield more precise estimates for $f(n)$.

3. An algebra of binomial type

The existence of a combinatorial interpretation of the coefficients $M_n(k)$ in the expansion

$$\left(\sum_{n=0}^{\infty} x^n/2^{\binom{n}{2}} n!\right)^k = \sum_{n=0}^{\infty} M_n(k) x^n/2^{\binom{n}{2}} n!$$

suggests the existence of an algebra of full binomial type with structure constants $B(n) = 2^{\binom{n}{2}} n!$ in the sense of [2]. This is equivalent to finding a locally finite partially ordered set P (said to be of *full binomial type*), satisfying the following conditions:

(a) In any segment $[x, y] = \{z \mid x \leqslant z \leqslant y\}$ of P (where $x \leqslant y$ in P), every maximal chain has the same length n. We call $[x, y]$ an *n-segment*.

(b) There exists an n-segment for every integer $n \geqslant 0$ and the number of maximal chains in any n-segment is $B(n) = 2^{\binom{n}{2}} n!$, (In particular, $B(1)$ must equal 1, further explaining the normalization $x' = 2^{1/2}x$ of Section 2.)

If such a partially ordered set P exists, then by [2] the value of $\zeta^k(x, y)$, where ζ is the zeta function of P, k is any integer and $[x, y]$ is any n-segment, depends only on k and n. We write $\zeta^k(x, y) = \zeta^k(n)$. Then again from [2],

$$\sum_{n=0}^{\infty} \zeta^k(n) x^n/B(n) = \left(\sum_{n=0}^{\infty} x^n/B(n) \right)^k .$$

Hence $\zeta^k(n) = M_n(k)$. In particular, the cardinality of any n-segment $[x, y]$ is $M_n(2)$, the number of labeled two-colored graphs with n vertices; while $\mu(x, y) = (-1)^n f(n)$, where μ is the Möbius function of P and $f(n)$ is the number of labeled acyclic digraphs with n vertices. The general theory developed in [2] provides a combinatorial interpretation of the coefficients of various other generating functions, such as $(\Sigma_{n=1}^{\infty} x^n/B(n))^k$ and $(2 - \Sigma_{n=0}^{\infty} x^n/B(n))^{-1}$.

Since $M_n(2)$ is the cardinality of an n-segment, this suggests taking elements of P to be properly two-colored graphs. We consider a somewhat more general situation.

Proposition 3.1. *Let V be an infinite vertex set, let q be a positive integer and let P_q be the set of all pairs (G, σ), where G is a function from all 2-sets $\{u, v\} \subseteq V$ $(u \neq v)$ into $\{0, 1, ..., q-1\}$ such that all but finitely many values of G are 0, and where $\sigma: V \to \{0, 1\}$ is a map satisfying the condition that if $G(\{u, v\}) > 0$ then $\sigma(u) \neq \sigma(v)$ and that $\Sigma_{u \in V}\sigma(u) < \infty$.*

If (G, σ) and (H, τ) are in P_q, define $(G, \sigma) \leqslant (H, \tau)$ if:

(a) *$\sigma(u) \leqslant \tau(u)$ for all $u \in V$, and*

(b) *If $\sigma(u) = \tau(u)$ and $\sigma(v) = \tau(v)$, then $G(\{u, v\}) = H(\{u, v\})$.*

Then P_q is a partially ordered set of full binomial type with structure constants $B(n) = n!\, q^{\binom{n}{2}}$.

Proof. If (H, τ) *covers* (G, σ) in P (i.e., if $(H, \tau) > (G, \sigma)$ and no (G', σ') satisfies $(H, \tau) > (G', \sigma') > (G, \sigma)$), then

$$\sum_{u \in V} \tau(u) = 1 + \sum_{u \in V} \sigma(u).$$

From this it follows that in every segment of P, all maximal chains have the same length.

In order to prove that an n-segment $S = [(G, \sigma), (H, \tau)]$ has $n!\, q^{\binom{n}{2}}$ maximal chains, it suffices to prove that (H, τ) covers exactly nq^{n-1} elements of S, for then the number of maximal chains in S will be $(nq^{n-1})((n-1)q^{n-2})\dots(2q^1)\cdot 1 = n!q^{\binom{n}{2}}$. Since S is an n-segment, there are precisely n vertices $v_1, v_2, \dots, v_n \in V$ such that $\sigma(v_i) = 0 < 1 = \tau(v_i)$. Suppose (H, τ) covers $(H', \tau') \in S$. Then τ' and τ agree on every $v \in V$ except for one v_i, say v_1, so $\tau'(v_1) = 0$, $\tau(v_1) = 1$. Suppose now $H'(\{u, v\}) > 0$, where we can assume $\tau'(u) = 0$, $\tau'(v) = 1$. If v is not some v_i, then $\sigma(u) = 0$, $\sigma(v) = 1$, so $H'(\{u, v\}) = G(\{u, v\})$. If $v = v_i$ $(2 \leqslant i \leqslant n)$ and u is not v_1, then $\tau(u) = 0$, $\tau(v) = 1$, so $H'(\{u, v\}) = H(\{u, v\})$. Hence $H'(\{u, v\})$ is completely determined unless $u = v_1$ and $v = v_i$, $2 \leqslant i \leqslant n$. In this case, each $H'(\{v_1, v_i\})$ can have any one of q values. Thus, there are n choices of v_1 and q choices for each $H'(\{v_1, v_i\})$, $2 \leqslant i \leqslant n$, giving a total of nq^{n-1} elements $(H', \tau') \in S$ covered by (H, τ).

Observe that when $q = 1$, condition (b) is vacuous, so P_1 is isomorphic to the lattice of finite subsets of V. When $q = 2$, we may think of $G(\{u, v\}) = 0$ or 1 depending on whether $\{u, v\}$ is not or is an edge of a graph on the vertex set V. Then σ is just a proper two-coloring of v with the colors 0 and 1, and the elements of P_2 consist of all properly two-colored graphs with vertex set V, finitely many edges and finitely many vertices colored 1. We remark that P_q is not a lattice unless $q = 1$.

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